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Low-symmetry spin Hamiltonian and crystal field tensors analysis: Fe3+ in natrolite

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Abstract

Electron paramagnetic resonance study of a natural single crystal of natrolite was carried out at the frequency ν = 36.772 GHz at room temperature. The angular dependence of the four symmetry-related spectra of Fe3+in the three crystallographic planes was fitted to a spin Hamiltonian (S = 5/2) of symmetry Ci. The rank 4 crystal field tensors at tetrahedral sites were calculated using the point-charge model to determine the principal axes orientations of their cubic and trigonal components. The analysis of zero-field splitting tensors and comparison with crystal field ones suggests that Fe3+ substitutes for Al3+ with no significant distortion of the coordination tetrahedron in natrolite. Comparison of data for several natural and synthetic crystals reveals that the 4-rank zero-field splitting tensor invariants for Fe3+ at the tetrahedral oxygen-coordinated sites are distinguishably smaller than those for Fe3+ at octahedral sites. Such comparative analysis may help to determine the substitutional sites in other crystals. © 2002 Elsevier Science (USA).

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Keywords

Crystal field, Low symmetry effect, Natrolite, Spin Hamiltonian, Tensor invariants